Butyl nitrate
928-45-0 | DTXSID70239143

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.82e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.71e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

Image not found
Butyl nitrate
Measured: 9.40e-03
Predicted: 8.82e-03

Image not found
Isobutyl nitrate
Measured: 1.12e-02
Predicted: 1.27e-02

Image not found
Nitric acid, 1-methylethyl ester
Measured: 3.47e-02
Predicted: 2.21e-02

Image not found
Isoamyl nitrate
Measured: 3.30e-03
Predicted: 3.33e-03

Image not found
Isoamyl nitrate
Measured: 3.30e-03
Predicted: 3.33e-03

Image not found
Amyl nitrate
Measured: 2.70e-03
Predicted: 3.21e-03